

The Strong-Coupling Polaron in Electromagnetic Fields

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Abstract

This paper is concerned with Fröhlich polarons subject to external electromagnetic fields in the limit of large electron-phonon coupling. To leading order in the coupling constant, $\sqrt{\alpha}$, the ground state energy is shown to be correctly given by the minimum of the Pekar functional including the electromagnetic fields, provided these fields in the Fröhlich model are scaled properly with α . As a corollary, the binding of two polarons in strong magnetic fields is obtained.

1 Introduction

The purpose of this paper is to determine the ground state energy $E(A, V, \alpha)$ of Fröhlich polarons subject to external electromagnetic fields $B = \operatorname{curl} A$ and $E = -\nabla V$ in the limit of large electron-phonon coupling, $\alpha \rightarrow \infty$. We show that $E(A, V, \alpha)$, to leading order in α , is given by the minimum of the Pekar functional including the electromagnetic fields, provided these fields in the Fröhlich model are scaled properly with α . Combining this result with our previous work on the binding of polarons in the Pekar-Tomasevich approximation, we prove here, for the first time, the existence of Fröhlich bipolarons in the presence of strong magnetic fields. These results were announced in [7].

The Fröhlich large polaron model without external fields has only one parameter, α , which describes the strength of the electron-phonon interaction. Hence the ground state energy $E(\alpha)$ is a function of α only, and since α is not small for many polar crystals, one is interested in the limit $\alpha \rightarrow \infty$. It had been conjectured long ago, and finally proved by Donsker and Varadhan [4], that

$$E(\alpha) = \alpha^2 E_P + o(\alpha^2), \quad (\alpha \rightarrow \infty), \quad (1)$$

where E_P is the minimum of the Pekar functional

$$\int |\nabla \varphi(x)|^2 dx - \iint \frac{|\varphi(x)|^2 |\varphi(y)|^2}{|x-y|} dx dy, \quad (2)$$

constrained by

$$\int |\varphi(x)|^2 dx = 1. \quad (3)$$

Statement (1) has later been reproved by Lieb and Thomas who also provided a bound on the error of the size $O(\alpha^{9/5})$ [11]. An interesting application of (1) is that it reduces the

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question of bipolaron formation, in the case $\alpha \gg 1$, to the analog question regarding the minimal energies of the Pekar and the Pekar-Tomasevich functionals. For these effective energy-functionals the binding of two polarons follows from a simple variational argument, provided the electron-electron repulsion constant belongs to the lower end of its physically admissible range. The minimizer of (2), (3), which is needed for the variational argument, is well-known to exist [9, 12]. This line of arguments, due to Miyao and Spohn [13], to our knowledge provides the only mathematically rigorous proof of the existence of bipolarons. While it assumes that $\alpha \gg 1$, numerical work suggest that $\alpha \geq 6.6$ may be sufficient for binding [15].

Whether or not polarons may form bound states if they are subject to external electromagnetic fields, e.g. constant magnetic fields, is an interesting open question. In view of [13, 7], this question calls for a generalization of (1) to systems including a magnetic field. In the present paper, for a large class of scalar and vector potentials V and A , respectively, we establish existence of a constant $C = C(A, V)$, such that

$$\alpha^2 E_P(A, V) \geq E(A_\alpha, V_\alpha, \alpha) \geq \alpha^2 E_P(A, V) - C\alpha^{9/5}, \quad (4)$$

where $A_\alpha(x) = \alpha A(\alpha x)$, $V_\alpha(x) = \alpha^2 V(\alpha x)$ and $E_P(A, V)$ is the infimum of the generalized Pekar functional

$$\int |D_A \varphi(x)|^2 + V(x)|\varphi(x)|^2 dx - \iint \frac{|\varphi(x)|^2 |\varphi(y)|^2}{|x-y|} dxdy \quad (5)$$

constrained by (3). Here $D_A = -i\nabla + A$. Non-scaled electromagnetic potentials become negligible in the limit $\alpha \rightarrow \infty$. In fact, we show that $\alpha^{-2} E(A, V, \alpha) \rightarrow E_P$ as $\alpha \rightarrow \infty$.

As explained above, (4) allows us to explore the possibility of bipolaron formation in the external fields A, V . The corresponding question concerning the effective theories of Pekar and Tomasevich with electromagnetic fields was studied in [7]. It was found, under the usual condition on the electron-electron repulsion (see above), that two polarons will bind provided the functional (5) attains its minimum, which is the case, e.g., for constant magnetic fields and $V \equiv 0$. This leads to our second main result, the binding of two polarons in strong constant magnetic fields, which follows from the more general Theorem 4.1, below. Of course it would be interesting to know whether or not the binding of polarons is enhanced by the presence of a magnetic field, as conjectured in [3]. This question is not addressed in the present paper.

The strong coupling result (1) was generalized in the recent work [1] to many-polaron systems, and one of us, Wellig, is presently extending this work to include magnetic fields. In work independent and simultaneous to ours, Frank and Geisinger have analyzed the ground state energy of the polaron for *fixed* $\alpha > 0$ in the limit of large, constant magnetic field, i.e., $A = B \wedge x/2$ and $|B| \rightarrow \infty$ [5]. They show that the ground state energy, both in the Fröhlich and the Pekar models, is given by $|B| - \frac{\alpha^2}{48} (\ln |B|)^2$ up to corrections of smaller order. The question of binding is not addressed, however, and seems to require a similar analysis of the ground state energy of the Pekar-Tomasevich model. For the binding of $N > 2$ polarons in the Pekar-Tomasevich model with and without external magnetic fields we refer to [8] and [2], respectively. For the thermodynamic stability, the non-binding, and the binding-unbinding transition of multipolaron systems the reader may consult the short review [6] and the references therein.

2 The Lower Bound

In this section we study the strong coupling limit of the minimal energy of the polaron subject to given external electric and magnetic fields. To exhibit the general validity of the method we shall allow for fairly general electric and magnetic potentials $V : \mathbb{R}^3 \rightarrow \mathbb{R}$ and $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$. We assume that $A_k \in L^2_{\text{loc}}(\mathbb{R}^3)$, $V \in L^1_{\text{loc}}(\mathbb{R}^3)$ and that for any $\varepsilon > 0$ and all $\varphi \in C_0^\infty(\mathbb{R}^3)$,

$$|\langle \varphi, V\varphi \rangle| \leq \varepsilon \|\nabla \varphi\|^2 + C_\varepsilon \|\varphi\|^2. \quad (6)$$

This is satisfied, e.g., when $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, see [14] or the proof of (22). Of course, here $\langle \varphi, V\varphi \rangle$ denotes a quadratic form defined by $\langle \varphi, V\varphi \rangle = \int V|\varphi|^2 dx$. Since $\langle D_A\varphi, D_A\varphi \rangle$ on $H_A^1(\mathbb{R}^3) := \{\varphi \in L^2(\mathbb{R}^3) \mid D_A\varphi \in L^2(\mathbb{R}^3)\}$ is a closed quadratic form with form core $C_0^\infty(\mathbb{R}^3)$, it follows, by the KLMN-theorem, that $\langle D_A\varphi, D_A\varphi \rangle + \langle \varphi, V\varphi \rangle$ is the quadratic form of a unique self-adjoint operator $D_A^2 + V$ whose form domain is $H_A^1(\mathbb{R}^3)$. Our assumptions allow for constant magnetic fields, the case in which we are most interested.

We shall next define the Fröhlich model associated with V and A through a quadratic form, which we shall prove to be semi-bounded. In this way the introduction of an ultraviolet cutoff is avoided. However, such a cutoff is used in the proof of semi-boundedness. The Hilbert space of the model in this section is the tensor product $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathcal{F}$, where \mathcal{F} denotes the symmetric Fock space over $L^2(\mathbb{R}^3)$, and the form domain is $\mathcal{Q} := H_A^1(\mathbb{R}^3) \otimes \mathcal{F}_0$ where

$$\mathcal{F}_0 := \{(\varphi^{(n)}) \in \mathcal{F} \mid \varphi^{(n)} \in C_0(\mathbb{R}^{3n}), \varphi^{(n)} = 0 \text{ for almost all } n\}.$$

We define a quadratic form H on \mathcal{Q} by

$$\begin{aligned} H(\psi) &:= \langle \psi, (D_A^2 + V)\psi \rangle + N(\psi) + \sqrt{\alpha}W(\psi) \\ N(\psi) &:= \int \|a(k)\psi\|^2 dk \end{aligned} \quad (7)$$

$$W(\psi) := \frac{1}{\sqrt{2\pi}} \int \frac{dk}{|k|} (\langle \psi, e^{ikx}a(k)\psi \rangle + \langle e^{ikx}a(k)\psi, \psi \rangle). \quad (8)$$

Note that $a(k)$ is a well-defined, linear operator on \mathcal{F}_0 but $a^*(k)$ is not and neither is $\int |k|^{-1}e^{-ikx}a^*(k)dk$, because $|k|^{-1}e^{-ikx}$ is not square integrable with respect to k . The Theorems 3.1 and 3.2 in the next section relate

$$E(A, V, \alpha) := \inf\{H(\psi) \mid \psi \in \mathcal{Q}, \|\psi\| = 1\}$$

to the minimum, $E_P(A, V)$, of the Pekar functional (5) on the unit sphere $\|\varphi\| = 1$. For the proofs it is convenient to introduce a coupling constant α in the Pekar functional and to define $E_P(A, V, \alpha)$ as the minimum of

$$\mathcal{E}_\alpha(A, V, \varphi) = \int |D_A\varphi(x)|^2 + V(x)|\varphi(x)|^2 dx - \alpha \iint \frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|} dx dy$$

with the constraint $\|\varphi\| = 1$. We set $\mathcal{E}(\varphi) = \mathcal{E}_{\alpha=1}(0, 0, \varphi)$, which is the Pekar functional (2). It is easy to check that

$$E_P(A_\alpha, V_\alpha, \alpha) = \alpha^2 E_P(A, V) \quad (9)$$

where $A_\alpha(x) = \alpha A(\alpha x)$, $V_\alpha(x) = \alpha^2 V(\alpha x)$.

The number $E_P(A, V, \alpha)$ is finite because $E_P(A, V, \alpha) \geq E_P(0, V, \alpha)$, by the diamagnetic inequality [10], and $E_P(0, V, \alpha) > -\infty$ by assumption on V and a simple exercise using the Hölder and Hardy inequalities. Our key result is the following lower bound on $E(A, V, \alpha)$:

Proposition 2.1. *Suppose that A, V satisfy the assumptions described above and $\beta = 1 - \alpha^{-1/5}$. Then*

$$E(A, V, \alpha) \geq \beta E_P(A, \beta^{-1}V, \alpha\beta^{-2}) - O(\alpha^{9/5}), \quad (\alpha \rightarrow \infty), \quad (10)$$

the error bound being independent of A and V .

The proof of Proposition 2.1 is done in several steps following [11]. Some of them can be taken over verbatim upon the substitution $-i\nabla_x \rightarrow -i\nabla_x + A(x)$. Surprisingly, the translation invariance that seemed to play some role in [11] is not needed for the arguments to work. For the convenience of the reader we at least sketch the main ideas.

To begin with, we introduce a quadratic form $\langle \psi, H_\Lambda \psi \rangle$ on \mathcal{Q} in terms of

$$H_\Lambda := \beta D_A^2 + V + N_{B_\Lambda} + \frac{\sqrt{\alpha}}{\sqrt{2\pi}} \int_{B_\Lambda} \frac{dk}{|k|} (e^{ikx} a(k) + e^{-ikx} a^*(k))$$

where $\beta := 1 - \frac{8\alpha}{\pi\Lambda}$, $B_\Lambda := \{k \in \mathbb{R}^3 : |k| \leq \Lambda\}$ and generally, for subsets $\Omega \subset \mathbb{R}^3$,

$$N_\Omega := \int_\Omega a^*(k) a(k) dk.$$

The quadratic form H_Λ is bounded below provided that $\Lambda > 8\alpha/\pi$.

Lemma 2.2. *In the sense of quadratic forms on \mathcal{Q} , for any $\Lambda > 0$,*

$$H(\psi) \geq \langle \psi, (H_\Lambda - \frac{1}{2})\psi \rangle.$$

This lemma, without electromagnetic fields, is due to Lieb and Thomas [11]. Its proof is based on the operator identity

$$e^{ikx} a(k) = \sum_{\ell=1}^3 \left[D_{A,\ell}, \frac{k_\ell}{|k|^2} e^{ikx} a(k) \right] \quad (11)$$

where $D_{A,\ell} = -i\partial_{x_\ell} + A_\ell(x)$. Obviously, $A(x)$ plays no role in (11) as it drops out of the commutator, but we need it for the estimates to follow. For any given $\Lambda > 0$ and $x \in \mathbb{R}^3$ we define the Fock space operators

$$\begin{aligned} \phi_\Lambda(x) &:= \frac{1}{\sqrt{2\pi}} \int_{B_\Lambda} (e^{ikx} a(k) + e^{-ikx} a^*(k)) \frac{dk}{|k|} \\ Z_\ell(x) &:= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}^3 \setminus B_\Lambda} \frac{k_\ell}{|k|^3} e^{ikx} a(k) dk \end{aligned}$$

and we extend them to operators ϕ_Λ, Z_ℓ on \mathcal{H} by setting $(\phi_\Lambda \psi)(x) := \phi_\Lambda(x)\psi(x)$, $(Z_\ell \psi)(x) := Z_\ell(x)\psi(x)$ for $\psi \in \mathcal{H} \simeq L^2(\mathbb{R}^3; \mathcal{F})$. Then, by (11), the electron-phonon interaction W can be written as

$$W(\psi) = \left\langle \psi, \left(\phi_\Lambda + \sum_{\ell=1}^3 [D_{A,\ell}, Z_\ell - Z_\ell^*] \right) \psi \right\rangle. \quad (12)$$

Following [11] one now shows that

$$\sqrt{\alpha} \sum_{\ell=1}^3 [D_{A,\ell}, Z_\ell - Z_\ell^*] \geq -\frac{8\alpha}{\pi\Lambda} D_A^2 - (N - N_{B_\Lambda}) - \frac{1}{2}. \quad (13)$$

The Lemma 2.2 follows from (12) and (13).

The next step is to *localize the electron* in a box of side length L . To this end we define the localization function

$$\varphi(x) = \begin{cases} \prod_{j=1}^3 \cos(\frac{\pi}{L}x_j) & \text{for } |x_j| \leq L/2, \\ 0 & \text{otherwise,} \end{cases}$$

and $\varphi_y(x) := \varphi(x - y)$.

Lemma 2.3. *For given $\Delta E > 0$ define $L > 0$ by $3\beta(\frac{\pi}{L})^2 = \Delta E$ and let φ be as above. Then for every non-vanishing $\psi \in \mathcal{Q}$ there exists a point $y \in \mathbb{R}^3$, such that $\varphi_y\psi \neq 0$ and*

$$\langle \varphi_y\psi, H_\Lambda \varphi_y\psi \rangle \leq (E + \Delta E) \|\varphi_y\psi\|^2,$$

where $E := \langle \psi, H_\Lambda \psi \rangle$.

Proof. Using $\varphi_y D_A^2 \varphi_y = D_A \varphi_y^2 D_A + \varphi_y(-\Delta \varphi_y)$ and $\beta \varphi_y(-\Delta \varphi_y) = \varphi_y^2 \Delta E$ one shows that

$$\int \langle \varphi_y\psi, (H_\Lambda - E - \Delta E)\varphi_y\psi \rangle dy = 0,$$

which proves the lemma. \square

The Lemma 2.3 is to be read as a bound on $E = \langle \psi, H_\Lambda \psi \rangle$ from below: using that H_Λ is translation invariant, except for the terms involving A and V , it implies together with Lemma 2.2 that

$$E(A, V, \alpha) \geq \inf_{y \in \mathbb{R}^3} \left(\inf_{\psi \in \mathcal{Q}_L, \|\psi\|=1} \langle \psi, H_{\Lambda,y} \psi \rangle \right) - \Delta E - \frac{1}{2}, \quad (14)$$

where $H_{\Lambda,y}$ is defined in terms of the shifted potentials $A_y(x) = A(x + y)$ and $V_y(x) = V(x + y)$, $\mathcal{Q}_L := (L^2(C_L) \otimes \mathcal{F}) \cap \mathcal{Q}$, and $C_L = \text{supp}(\varphi) \subset \mathbb{R}^3$ is the cube of side length L centered at the origin.

The next step is the passage to *block modes*. For given $P > 0$ and $n \in \mathbb{Z}^3$ we define

$$\begin{aligned} B(n) &:= \{k \in B_\Lambda \mid |k_i - n_i P| \leq P/2\}, \\ \Lambda_P &:= \{n \in \mathbb{Z}^3 \mid B(n) \neq \emptyset\}. \end{aligned}$$

In each set $B(n)$ we pick a point k_n , to be specified later, and we define block annihilation and creation operators a_n and a_n^* by

$$a_n := \frac{1}{M_n} \int_{B(n)} \frac{dk}{|k|} a(k), \quad M_n = \left(\int_{B(n)} \frac{dk}{|k|^2} \right)^{1/2}.$$

For given $\delta > 0$ we define the block Hamiltonian

$$\begin{aligned} H_{\Lambda,y}^{block} &:= \beta D_{A_y}^2 + V_y + (1 - \delta) \sum_{n \in \Lambda_P} a_n^* a_n \\ &\quad + \frac{\sqrt{\alpha}}{\sqrt{2}\pi} \sum_{n \in \Lambda_P} M_n (e^{ik_n x} a_n + e^{-ik_n x} a_n^*), \end{aligned}$$

and we set $H_\Lambda^{block} := H_{\Lambda,0}^{block}$. The reason for introducing block modes is well explained in [11] and related to (18).

Lemma 2.4. *In the sense of quadratic forms in \mathcal{Q}_L , for all (k_n) ,*

$$H_{\Lambda,y} \geq H_{\Lambda,y}^{block} - \frac{9\alpha P^2 L^2 \Lambda}{2\pi\delta}.$$

Proof. For each $n \in \Lambda_P$, by a completion of squares w.r.t. $a(k)$ and $a^*(k)$ we find, in the sense of quadratic forms in \mathcal{Q}_L ,

$$\begin{aligned} & \delta N_{B(n)} + \frac{\sqrt{\alpha}}{\sqrt{2\pi}} \int_{B(n)} \frac{dk}{|k|} (e^{ikx} a(k) + e^{-ikx} a^*(k)) \\ & \geq \frac{\sqrt{\alpha}}{\sqrt{2\pi}} \int_{B(n)} \frac{dk}{|k|} (e^{ik_n x} a(k) + e^{-ik_n x} a^*(k)) - \frac{\alpha}{2\pi^2 \delta} \int_{B(n)} \frac{dk}{|k|^2} |e^{ikx} - e^{ik_n x}|^2 \\ & \geq \frac{\sqrt{\alpha}}{\sqrt{2\pi}} M_n (e^{ik_n x} a_n + e^{-ik_n x} a_n^*) - \frac{\alpha}{2\pi^2 \delta} \left(\frac{3}{2} PL\right)^2 \int_{B(n)} \frac{dk}{|k|^2}, \end{aligned} \quad (15)$$

where we used the definition of a_n and that

$$|e^{ikx} - e^{ik_n x}| \leq \frac{3}{2} PL, \quad \text{for } x \in C_L, \quad k \in B(n).$$

After summing (15) with respect to $n \in \Lambda_P$, the lemma follows from $\int_{B_\Lambda} |k|^{-2} dk = 4\pi\Lambda$ and from $a_n^* a_n \leq N_{B(n)}$. \square

We now use Lemma 2.4 to bound (14) from below and then we replace \mathcal{Q}_L by \mathcal{Q} . This leads to

$$E(A, V, \alpha) \geq \inf_{\psi \in \mathcal{Q}, \|\psi\|=1} \sup_{k_n} \left\langle \psi, H_{\Lambda,y}^{block} \psi \right\rangle - \frac{9\alpha P^2 L^2 \Lambda}{2\pi\delta} - \Delta E - \frac{1}{2}. \quad (16)$$

Recall that L depends on ΔE . It remains to compare $\left\langle \psi, H_{\Lambda,y}^{block} \psi \right\rangle$ with the minimum of the Pekar functional. This will be done in the proof of the following lemma using coherent states.

Lemma 2.5. *Let $\mu = \alpha\beta^{-1}(1-\delta)^{-1}$. Then for every normalized $\psi \in \mathcal{Q}$ and every $y \in \mathbb{R}^3$,*

$$\sup_{k_n} \left\langle \psi, H_{\Lambda,y}^{block} \psi \right\rangle \geq \beta E_P(A, V, \mu) - |\Lambda_P|.$$

Proof. Since $E_P(A_y, V_y, \mu)$ is independent of y it suffices to prove the asserted inequality without the y -shift in the block Hamiltonian. Let $M = \text{span}\{|\cdot|^{-1} \chi_{B(n)} \mid n \in \Lambda_P\}$, which is a finite dimensional subspace of $L^2(\mathbb{R}^3)$. From $L^2(\mathbb{R}^3) = M \oplus M^\perp$ it follows that \mathcal{F} is isomorphic to $\mathcal{F}(M) \otimes \mathcal{F}(M^\perp)$ with the isomorphism given by

$$\begin{aligned} \Omega & \mapsto \Omega \otimes \Omega \\ a^*(h) & \mapsto a^*(h_1) \otimes 1 + 1 \otimes a^*(h_2) \end{aligned}$$

where h_1 and h_2 are the orthogonal projections of h onto M and M^\perp respectively. Here Ω denotes the normalized vacuum in any Fock space. Note that

$$\mathcal{F}(M) = \overline{\text{span}} \left\{ \prod_{n \in \Lambda_P} (a_n^*)^{m_n} \Omega \mid m_n \in \mathbb{N} \right\} \quad (17)$$

where $\overline{\text{span}}$ denotes the closure of the span. With respect to the factorization $\mathcal{H} = \mathcal{H}_M \otimes \mathcal{F}(M^\perp)$ where $\mathcal{H}_M = L^2(\mathbb{R}^3) \otimes \mathcal{F}(M)$, the block Hamiltonian is of the form $H_\Lambda^{\text{block}} \otimes 1$. To bound $H_\Lambda^{\text{block}} \otimes 1$ on $\mathcal{H}_M \otimes \mathcal{F}(M^\perp)$ from below we introduce coherent states $|z\rangle \in \mathcal{F}(M)$ for given $z = (z_n)_{n \in \Lambda_P}$, $z_n \in \mathbb{C}$, by

$$|z\rangle := \prod_{n \in \Lambda_P} e^{z_n a_n^* - \bar{z}_n a_n} \Omega.$$

Clearly, $\langle z, z \rangle = 1$ and it is easy to check that $a_n|z\rangle = z_n|z\rangle$. On $\mathcal{F}(M)$, in the sense of weak integrals,

$$\begin{aligned} \int dz |z\rangle \langle z| &= 1, \\ \int dz (|z_n|^2 - 1) |z\rangle \langle z| &= a_n^* a_n, \end{aligned} \tag{18}$$

where $\int dz := \prod_{n \in \Lambda_P} \frac{1}{\pi} \int dx_n dy_n$. The second equation follows from $a_n^* a_n = a_n a_n^* - 1$ and from the first one. Now suppose that $\psi \in \mathcal{Q}$ and let $\psi_z(x) = \langle z, \psi(x) \rangle$. Then $\psi_z \in L^2(\mathbb{R}^3) \otimes \mathcal{F}(M^\perp)$ and

$$\langle \psi, H_\Lambda^{\text{block}} \psi \rangle = \int dz \langle \psi_z, (h_z \otimes 1) \psi_z \rangle$$

where h_z denotes the Schrödinger operator in $L^2(\mathbb{R}^3)$ given by

$$h_z = \beta D_A^2 + V + (1 - \delta) \sum_{n \in \Lambda_P} (|z_n|^2 - 1) + \frac{\sqrt{\alpha}}{\sqrt{2}\pi} \sum_{n \in \Lambda_P} M_n (z_n e^{ik_n x} + \overline{z_n} e^{-ik_n x}).$$

Let $\widehat{\rho}_z(k) := \langle \psi_z, e^{-ikx} \psi_z \rangle$ be the Fourier transform of $\rho_z(x) = |\psi_z(x)|^2$. By completion of the square w.r.to z_n and $\overline{z_n}$ it follows that

$$\begin{aligned} \sup_{k_n} \int dz \langle \psi_z, (h_z \otimes 1) \psi_z \rangle &\geq \int dz \beta \|D_A \psi_z\|^2 + \langle \psi_z, V \psi_z \rangle - \frac{\alpha}{2\pi^2(1-\delta)} \int dz \int_{B_\Lambda} \frac{dk}{|k|^2} |\widehat{\rho}_z(k)|^2 \frac{1}{\|\psi_z\|^2} - |\Lambda_P| \\ &\geq \int dz \left(\beta \|D_A \psi_z\|^2 + \langle \psi_z, V \psi_z \rangle - \frac{\alpha}{(1-\delta)\|\psi_z\|^2} \int \frac{\rho_z(x)\rho_z(y)}{|x-y|} dx dy \right) - |\Lambda_P|. \end{aligned}$$

The integrand is readily recognized as

$$\beta \|\psi_z\|^2 \mathcal{E}_\mu(A, \beta^{-1}V, \psi_z/\|\psi_z\|),$$

with coupling constant $\mu := \alpha\beta^{-1}(1-\delta)^{-1}$. Its minimum is

$$\beta \|\psi_z\|^2 E_P(A, \beta^{-1}V, \mu).$$

Since $\int \|\psi_z\|^2 dz = 1$, the proof of the lemma is complete. \square

Proof of Proposition 2.1. By (16) and Lemma 2.5 it follows that

$$E(A, V, \alpha) \geq \beta E_P(A, \beta^{-1}V, \mu) - |\Lambda_P| - \frac{9\alpha P^2 L^2 \Lambda}{2\pi\delta} - \Delta E - \frac{1}{2}$$

where $\beta = 1 - \frac{8\alpha}{\pi\Lambda}$, $\mu = \alpha\beta^{-1}(1-\delta)^{-1}$ and $L^2 = \pi^2 3\beta/\Delta E$. Λ, δ, P and ΔE are free parameters. We choose $\Lambda = \frac{8}{\pi}\alpha^{6/5}$, $\delta = \alpha^{-1/5}$, $P = \alpha^{3/5}$ and $\Delta E = \alpha^{9/5}$. Then $\beta = 1 - \delta$ and hence the proposition follows. \square

3 The Strong Coupling Limit

Equipped with Proposition 2.1 we can turn to the proofs of the results described in the introduction in the more precise forms of Theorems 3.1 and 3.2, below.

Theorem 3.1. *Suppose the potentials A and V satisfy the assumptions of Proposition 2.1, $A_\alpha(x) := \alpha A(\alpha x)$ and $V_\alpha(x) := \alpha^2 V(\alpha x)$. Then there exists a constant $C = C(A, V)$ such that for $\alpha > 0$ large enough,*

$$\alpha^2 E_P(A, V) \geq E(A_\alpha, V_\alpha, \alpha) \geq \alpha^2 E_P(A, V) - C\alpha^{9/5}.$$

Proof. The first inequality follows from the well-known $E_P \geq E$, see the proof of (30), and from the scaling property (9) of E_P . Using Proposition 2.1 and (9), we see that

$$E(A_\alpha, V_\alpha, \alpha) \geq \alpha^2 \beta E_P(A, \beta^{-1}V, \beta^{-2}) - O(\alpha^{9/5}) \quad (19)$$

where $\beta = 1 - \alpha^{-1/5}$ and where the function $\lambda \mapsto E_P(A, \lambda V, \lambda^2)$, as an infimum of concave functions, is concave. Therefore it has one-sided derivatives, which implies that

$$E_P(A, \beta^{-1}V, \beta^{-2}) \geq E_P(A, V) - O(\alpha^{-1/5}). \quad (20)$$

Combining (19) and (20) the second inequality from Theorem 3.1 follows. \square

Theorem 3.2.

- (a) *If $A \in L_{\text{loc}}^3(\mathbb{R}^3)$ and $V \in L_{\text{loc}}^{3/2}(\mathbb{R}^3)$ with (6), then $\alpha^{-2}E(A, V, \alpha) \rightarrow E_P$ as $\alpha \rightarrow \infty$.*
- (b) *If $A = (B \wedge x)/2$ and $V \in L^{5/3}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, then*

$$\frac{E(A, V, \alpha)}{\alpha^2} = E_P + O(\alpha^{-1/5}), \quad (\alpha \rightarrow \infty).$$

The fact that non-scaled fields A, V should become negligible in the limit $\alpha \rightarrow \infty$ is seen as follows: by Proposition 2.1 and by (9), $\alpha^{-2}E(A, V, \alpha)$ is bounded from above and from below by

$$E_P(A_{\alpha^{-1}}, V_{\alpha^{-1}}) \geq \frac{E(A, V, \alpha)}{\alpha^2} \geq \beta E_P(A_{\alpha^{-1}}, \beta^{-1}V_{\alpha^{-1}}, \beta^{-2}) - O(\alpha^{-1/5}), \quad (21)$$

where $A_{\alpha^{-1}}(x) = \alpha^{-1}A(x/\alpha)$ and $V_{\alpha^{-1}}(x) = \alpha^{-2}V(x/\alpha)$. In the limit $\alpha \rightarrow \infty$ these fields are vanishing in the sense of the following lemma. The theorem will thus follow from parts (b) and (c) of Lemma 3.4 below. As a preparation we need:

Lemma 3.3. (i) *Suppose $A \in L_{\text{loc}}^3(\mathbb{R}^3)$ and $V \in L_{\text{loc}}^{3/2}(\mathbb{R}^3)$. Then*

$$\begin{aligned} A_{\alpha^{-1}} &\rightarrow 0 \quad (\alpha \rightarrow \infty) \quad \text{in } L_{\text{loc}}^2(\mathbb{R}^3), \\ V_{\alpha^{-1}} &\rightarrow 0 \quad (\alpha \rightarrow \infty) \quad \text{in } L_{\text{loc}}^1(\mathbb{R}^3). \end{aligned}$$

(ii) *If $V = V_1 + V_2 \in L^{5/3}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, then for all $\varphi \in H^1(\mathbb{R}^3)$*

$$|\langle \varphi, V\varphi \rangle| \leq C\|V_1\|_{5/3}\|\varphi\|_{H^1}^2 + \|V_2\|_\infty\|\varphi\|^2. \quad (22)$$

In particular, V is infinitesimally form bounded w.r.to $-\Delta$.

Proof. (i) Let $\Omega \subset \mathbb{R}^3$ be compact. By Cauchy-Schwarz,

$$\begin{aligned} \int_{\Omega} |A_{\alpha^{-1}}(x)|^2 dx &= \alpha \int_{\alpha^{-1}\Omega} |A(x)|^2 dx \\ &\leq \left(\int |A(x)|^3 \chi_{\alpha^{-1}\Omega}(x) dx \right)^{2/3} |\Omega|^{1/3} \rightarrow 0 \quad (\alpha \rightarrow \infty). \end{aligned}$$

The second statement of (i) is proved similarly.

In statement (ii) the contribution due to V_2 is obvious. Let us assume that $V = V_1 \in L^{5/3}(\mathbb{R}^3)$. By Hölder's inequality $|\langle \varphi, V\varphi \rangle| \leq \|V\|_{5/3} \|\varphi\|_5^2$ and

$$\int |\varphi|^5 dx \leq \|\varphi\|^{1/2} \left(\int |\varphi|^6 dx \right)^{3/4}. \quad (23)$$

Using the general inequality $ab \leq p^{-1}a^p + q^{-1}b^q$ with $p = 10$ and $q = 10/9$ we obtain

$$\|\varphi\|_5^2 \leq \|\varphi\|^{1/5} \|\varphi\|_6^{9/5} \leq \frac{1}{10} \|\varphi\|^2 + \frac{9}{10} \|\varphi\|_6^2.$$

Statement (ii) now follows from the Sobolev inequality $\|\varphi\|_6^2 \leq C \|\nabla \varphi\|^2$. The infinitesimal form bound follows from the fact that the norm of the $L^{5/3}$ -part of V can be chosen arbitrarily small. \square

Lemma 3.4. *Let A, V be real-valued potentials satisfying the hypothesis of Lemma 3.3 (i), and suppose that (6) holds. If $\lim_{\alpha \rightarrow \infty} \lambda(\alpha) = 1$, then*

- (a) $\lim_{\alpha \rightarrow \infty} \mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi) = \mathcal{E}(\varphi)$ for all $\varphi \in C_0^\infty(\mathbb{R}^3)$,
- (b) $\lim_{\alpha \rightarrow \infty} E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) = E_P$.

If $A = (B \wedge x)/2$, $V \in L^{5/3}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and $\lim_{\alpha \rightarrow \infty} \lambda(\alpha) = 1$, then

- (c) $E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) = \lambda^4 E_P + O(\alpha^{-1/5}), \quad (\alpha \rightarrow \infty)$.

Proof. (a) For $\varphi \in C_0^\infty(\mathbb{R}^3)$, Lemma 3.3 implies that $\|A_{\alpha^{-1}}\varphi\| \rightarrow 0$ and $\langle \varphi, V_{\alpha^{-1}}\varphi \rangle \rightarrow 0$ as $\alpha \rightarrow \infty$. This proves (a).

(b) For any normalized $\varphi \in C_0^\infty(\mathbb{R}^3)$, by (a),

$$\limsup_{\alpha \rightarrow \infty} E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) \leq \limsup_{\alpha \rightarrow \infty} \mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi) = \mathcal{E}(\varphi).$$

This implies that $\limsup_{\alpha \rightarrow \infty} E_P(A, \lambda V, \lambda^2 \alpha) \alpha^{-2} \leq E_P$.

For (b) it remains to prove that $\liminf_{\alpha \rightarrow \infty} E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) \geq E_P$. By the hypothesis on V , for any $\varepsilon > 0$ and any normalized $\varphi \in C_0^\infty(\mathbb{R}^3)$,

$$|\langle \varphi, V_{\alpha^{-1}}\varphi \rangle| \leq \varepsilon \|\nabla \varphi\|^2 + \frac{C_\varepsilon}{\alpha^2}. \quad (24)$$

From (24), the diamagnetic inequality and the scaling property of E_P , it follows that

$$\mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi) \geq (1 - \lambda \varepsilon) E_P(0, 0, \lambda^2 / (1 - \lambda \varepsilon)) - \lambda \frac{C_\varepsilon}{\alpha^2} \quad (25)$$

$$\geq \frac{\lambda^4}{(1 - \lambda \varepsilon)} E_P - \lambda \frac{C_\varepsilon}{\alpha^2}, \quad (26)$$

and hence that

$$E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) \geq \frac{\lambda^4}{(1 - \lambda\varepsilon)} E_P - \lambda \frac{C_\varepsilon}{\alpha^2}.$$

Now letting first $\alpha \rightarrow \infty$ and then $\varepsilon \rightarrow 0$, the desired lower bound is obtained.

The proof of the lower bound in (c) is similar to the proof of the lower bound in (b), the main difference being that we now have (22) from Lemma 3.3, which implies that

$$|\langle \varphi, V_{\alpha^{-1}}\varphi \rangle| \leq C\alpha^{-1/5}(\|\varphi\|^2 + \|\nabla|\varphi|\|^2) \quad (27)$$

with some $C > 0$ that is independent of α and φ . By the diamagnetic inequality and by (27), for any normalized $\varphi \in C_0^\infty(\mathbb{R}^3)$,

$$\begin{aligned} \mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi) &\geq \mathcal{E}_{\lambda^2}(0, 0, |\varphi|) - C\lambda\alpha^{-1/5}(1 + \|\nabla|\varphi|\|^2) \\ &\geq (1 - C\lambda\alpha^{-1/5})E_P(0, 0, \frac{\lambda^2}{1 - C\lambda\alpha^{-1/5}}) - C\lambda\alpha^{-1/5} \\ &= \frac{\lambda^4}{1 - C\lambda\alpha^{-1/5}}E_P - C\lambda\alpha^{-1/5}. \end{aligned}$$

Hence $E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) \geq \lambda^4 E_P - O(\alpha^{-1/5})$.

It remains to prove the upper bound on $E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2)$ in (c). To this end let φ_0 be a (real-valued) minimizer of the Pekar functional [9], i.e. $\mathcal{E}(\varphi_0) = E_P$ and let φ_λ be scaled in such a way that $\mathcal{E}_{\lambda^2}(\varphi_\lambda) = \lambda^4 \mathcal{E}(\varphi_0)$. Then

$$\begin{aligned} E_P(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \lambda^2) &\leq \mathcal{E}_{\lambda^2}(A_{\alpha^{-1}}, \lambda V_{\alpha^{-1}}, \varphi_\lambda) \\ &= \lambda^4 E_P + \|A_{\alpha^{-1}}\varphi_\lambda\|^2 + \lambda \langle \varphi_\lambda, V_{\alpha^{-1}}\varphi_\lambda \rangle \\ &= \lambda^4 E_P + O(\alpha^{-1/5}). \end{aligned}$$

We have used that $\operatorname{Re} \langle -i\nabla\varphi_\lambda, A_{\alpha^{-1}}\varphi_\lambda \rangle = 0$, since φ_λ is real-valued, and (22) from Lemma 3.3

□

4 Existence of Bipolarons

Let A, V be vector and scalar potentials, respectively, satisfying the assumptions of the Section 2. Let $\alpha, U > 0$. We define a two-body Hamiltonian $H_U^{A,V}$ on $L^2(\mathbb{R}^6)$ by

$$H_U^{A,V} := (D_A^2 + V) \otimes 1 + 1 \otimes (D_A^2 + V) + UV_C \quad (28)$$

where $V_C(x, y) := |x - y|^{-1}$. More precisely, we define $H_U^{A,V}$ in terms of the quadratic form given by the right hand side of (28) on $C_0^\infty(\mathbb{R}^6)$. Its form domain will be denoted by $H_A^1(\mathbb{R}^6)$.

In the two-polaron model of Fröhlich, the minimal energy, $E_2(A, V, U, \alpha)$ of two electrons in a polar crystal is the infimum of the quadratic form

$$\langle \psi, (H_U^{A,V} \otimes 1)\psi \rangle + N(\psi) + \sqrt{\alpha}W_2(\psi), \quad (29)$$

whose domain is the intersection of $H_A^1(\mathbb{R}^6) \otimes \mathcal{F}_0$ with the unit sphere of the Hilbert space $L^2(\mathbb{R}^6) \otimes \mathcal{F}$. Here $N(\psi)$ and $W_2(\psi)$ are defined by expressions similar to (7) and (8), the main difference being that e^{ikx} in (8) becomes $e^{ikx_1} + e^{ikx_2}$ in $W_2(\psi)$.

In the two-polaron model of Pekar and Tomasevich the minimal energy, $E_{PT}(A, V, U, \alpha)$ of two electrons in a polar crystal is the infimum of the functional

$$\left\langle \varphi, H_U^{A,V} \varphi \right\rangle - \alpha \iint \frac{\rho(x)\rho(y)}{|x-y|} dx dy$$

on the L^2 -unit sphere of $H_A^1(\mathbb{R}^6)$, where $\rho(x) := \int (|\varphi(x, y)|^2 + |\varphi(y, x)|^2) dy$. For any fixed $\varphi \in L^2(\mathbb{R}^6) \cap H_A^1(\mathbb{R}^6)$, $\|\varphi\| = 1$, and corresponding density ρ the identity

$$\inf_{\|\eta\|=1} (N(\varphi \otimes \eta) + \sqrt{\alpha} W_2(\varphi \otimes \eta)) = -\alpha \iint \frac{\rho(x)\rho(y)}{|x-y|} dx dy$$

holds. By choosing $\psi = \varphi \otimes \eta$ in (29) it follows that

$$E_{PT}(A, V, U, \alpha) \geq E_2(A, V, U, \alpha), \quad (30)$$

which, together with Theorem 3.1 and the results of [7] enables us to prove the following theorem on the *binding of polarons*:

Theorem 4.1. *Suppose $A, V \in L^2_{\text{loc}}(\mathbb{R}^3)$ and that V is infinitesimally operator bounded w.r.to Δ . Let $A_\alpha(x) = \alpha A(\alpha x)$ and $V_\alpha(x) = \alpha^2 V(\alpha x)$. If the Pekar functional (5) attains its minimum, then there exists $u_{A,V} > 2$ such that for $U < \alpha u_{A,V}$ and α large enough*

$$2E(A_\alpha, V_\alpha, \alpha) > E_2(A_\alpha, V_\alpha, U, \alpha).$$

Proof. Let $U = \alpha u$. By a simple scaling argument

$$E_{PT}(A_\alpha, V_\alpha, \alpha u, \alpha) = \alpha^2 E_{PT}(A, V, u, 1), \quad (31)$$

which is analogous to (9). By Theorem 3.1 of [7] there exists $u_{A,V} > 2$ such that for $u < u_{A,V}$,

$$2E_P(A, V) > E_{PT}(A, V, u, 1). \quad (32)$$

From Theorem 3.1, (32), (31), and (30) it follows that, for α large enough,

$$\begin{aligned} 2\alpha^{-2} E(A_\alpha, V_\alpha, \alpha) &= 2E_P(A, V) - o(1) \\ &> E_{PT}(A, V, u, 1) \\ &= \alpha^{-2} E_{PT}(A_\alpha, V_\alpha, \alpha u, \alpha) \\ &\geq \alpha^{-2} E_2(A_\alpha, V_\alpha, U, \alpha), \end{aligned}$$

which proves the theorem. \square

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